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How far can stochastic and deterministic views be reconciled?

Eric Bertin
Université de Lyon, Laboratoire de Physique, Ecole Normale Supérieure de Lyon, CNRS, 46 Allée d'Italie, F-69007 Lyon, France.

In this short note, we try to provide the reader with a brief pedagogical account of some similarities and differences between stochastic and deterministic processes. A short presentation of some basic notions related to the mathematical description of stochastic processes is also given. Our main aim is to illustrate the somehow surprising fact that the gap between the behaviour of stochastic and deterministic processes might, from a practical perspective, be much smaller than a priori expected.

Keywords: Stochastic processes, deterministic processes, transition to chaos, stochastic modelling

I. INTRODUCTION

Stochasticity and randomness appeared in physics nearly one century ago, with the emergence of statistical physics and quantum mechanics [1–3] –see also the paper by M. Le Bellac in this special issue. Randomness was at this stage essentially confined to the atomic scale, and a predictable behaviour was still assumed to hold at the macroscopic level. In the last fifty years, it was however recognized that even macroscopic and deterministic systems, with a small number of degrees of freedom, could behave in an unpredictable and apparently random manner; such systems have been called chaotic [4]. Stochasticity also appears nowadays as an essential ingredient in the dynamics of biological systems [5, 6], as witnessed by the present Special Issue on stochastic processes in cell biology.

In this note, we wish to illustrate, using a few simple mathematical examples, that chaotic and stochastic dynamics may look quite similar in certain cases, in spite of important conceptual differences. In addition, deterministic chaotic systems can in some situations be modelled by stochastic processes, as we shall see in the last section. This suggests that the gap between stochastic and deterministic (chaotic) dynamics might in some cases, from a practical perspective, be smaller than a priori expected.

The article is organised as follows. In section II, we present some basic notions on the mathematical formalism used to describe stochastic processes. In section III, we illustrate on a simple case the emergence of chaos in a deterministic system when varying a control parameter, as well as the notion of "chaotic walk", the deterministic analog to random walks. Finally, section IV discusses the possibility to use stochastic models in order to mimick the coarse-grained dynamics of a deterministic process.

II. BASIC NOTIONS ON STOCHASTIC PROCESSES

In this first section, we tentatively provide the reader with a brief and pedagogical presentation of the basic mathematical formalism describing stochastic processes, a knowledge useful to better grasp the essence of stochasticity. The interested reader is referred to standard textbooks, like Ref. [3], for more details.

A. Master equations

Let us start by considering the case of discrete time stochastic processes, that is stochastic processes with events randomly occuring between integer times $t = 0, 1, 2, ...$ The different configurations accessible to the process are labeled by an integer n. The process is described by transition probabilities $T(n' \to n)$ for all n, n', which gives the probability that the configuration is n at time $t+1$ given that it was n' at time t. Note that the configuration does not necessarily change at each step, the probability $T(n' \to n')$ is generally non zero.

The statistics of the process is described the probability $P_n(t)$ to be in state n at time t. This probability evolves according to the following discrete-time master equation

$$P_n(t+1) = \sum_{n'} T(n' \to n) P_{n'}(t) \tag{1}$$

which simply accounts for the balance of probabilities: the probability to be in state n at time $t+1$ results from all the transitions from any configurations n' to configuration n between times t and $t+1$, weighted by the transition probability $T(n' \to n)$ and by the probability $P_{n'}(t)$ to occupy configuration n' at time t. It is important to note

that we focus here on processes where no memory of previous configurations at time $t-1$, $t-2$,..., is present. Such processes are called "Markovian stochastic processes".

The continuous time case, which is the most commonly used in practical modelling, can be obtained from the discrete time case by taking the limit of infinitely short time steps. We thus choose very short time steps $\Delta t = dt$, instead of $\Delta t = 1$ as previously. It is then necessary to specify the behaviour of the transition probability with the time step dt. One expects in particular that the shorter the time interval dt, the smaller the transition probability to a different configuration in this interval. In other words, in a short time interval, the process "has not enough time" to change configuration, and most likely remains in the same one. A natural choice for the transition probabilities is thus

$$T(n' \to n) = W(n' \to n)\, dt \qquad \text{if} \quad n' \neq n \tag{2}$$

$$T(n \to n) = 1 - \sum_{n' \neq n} W(n' \to n)\, dt + \mathcal{O}(dt^2) \tag{3}$$

This choice indeed ensures that the different probabilities sum up to one, as expected. The new quantity $W(n' \to n)$ that has been introduced is called a "transition rate" (i.e., a transition probability per unit time). This quantity plays a key role in the description of continuous time stochastic processes.

The evolution of the probability $P_n(t)$ to be in configuration n at time t can be deduced from Eq. (1). Expanding $P_n(t+dt)$ to first order in dt yields

$$P_n(t+dt) = P_n(t) + \frac{dP_n}{dt}\, dt + \mathcal{O}(dt^2). \tag{4}$$

Gathering terms linear in dt, one finds the continuous time master equation

$$\frac{dP_n}{dt} = \sum_{n'} \Big[-W(n \to n')P_n(t) + W(n' \to n)P_{n'}(t) \Big]. \tag{5}$$

As a simple illustration, let us consider a process with only two configurations, $n = 1$ and 2. The transitions rates are $W(1 \to 2) = \alpha$ and $W(2 \to 1) = \beta$, see the left panel of Fig. 1. The master equation corresponds to the following set of equations

$$\frac{dP_1}{dt} = -\alpha P_1 + \beta P_2 \tag{6}$$

$$\frac{dP_2}{dt} = -\beta P_2 + \alpha P_1 \tag{7}$$

Taking into account the relation $P_1 + P_2 = 1$, these two equations are found to be equivalent, and can be reformulated as a single equation, namely

$$\frac{dP_1}{dt} = -(\alpha+\beta)P_1 + \beta. \tag{8}$$

The solution of this equation reads

$$P_1(t) = \frac{\beta}{\alpha+\beta} + \left(P_1(0) - \frac{\beta}{\alpha+\beta} \right) e^{-(\alpha+\beta)t} \tag{9}$$

where $P_1(0)$ is the initial value of the probability at time $t = 0$. One observes that $P_1(t)$ relaxes to the stationary value P_{st} as time elapses. An illustration of the behaviour of $P_1(t)$ is provided in the right panel of Fig. 1.

Coming back to the general (continuous time) master equation given in Eq. (5), it is interesting to try to characterize the stationary solutions, that is the solutions that are independent of time, corresponding to $dP_n/dt = 0$. It follows that for all n,

$$\sum_{n'} \left[-W(n \to n')P_n + W(n' \to n)P_{n'} \right] = 0. \tag{10}$$

A specific case of interest is when all terms in the sum are equal to zero, namely for all n and n'

$$-W(n \to n')P_n + W(n' \to n)P_{n'} = 0 \tag{11}$$

This situation is called detailed balance, and it turns out to be useful in practice to build models with desired stationary probabilities [3].

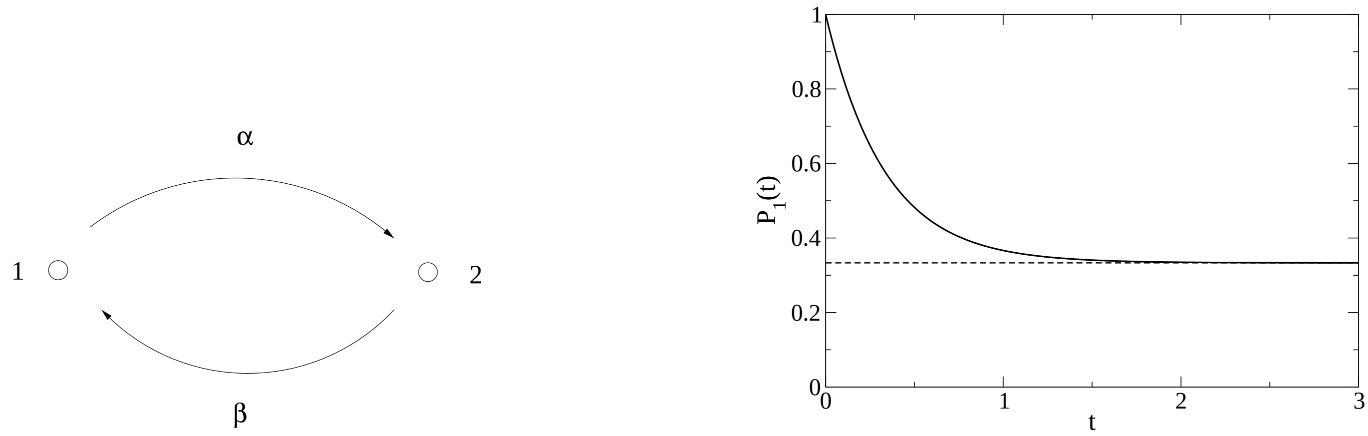

FIG. 1: Left: Illustration of the two-state model. Right: Relaxation of the probability $P_1(t)$ (full line) to its asymptotic equilibrium value (dashed line) in the two-state model (parameters: $\alpha = 2$, $\beta = 1$).

B. Example of the random walk on a line

The one-dimensional random walk, describing for instance the stochastic displacement of a particle on a line, can be defined as follows:

$$x_{t+\tau} = x_t + \epsilon_t, \qquad \epsilon_t = \pm a, \tag{12}$$

where τ is the constant time step. The values $+a$ and $-a$ are chosen at random with equal probabilities. In order to perform averages, one needs to use the so-called ensemble averages, corresponding to averages over many different realizations of the random walk. The average values obtained in this way are thus time-dependent, and should not be confused with time-averages.

It is easy to check that the average value of the position of the random walk is zero at all time, $\langle x_t \rangle = 0$, if the random walk initially starts from the position 0.

A more interesting quantity to characterize the statistical properties of the walk is the mean square displacement $\langle x_t^2 \rangle$. This quantity can be computed as follows. Taking the square of Eq. (12), one finds

$$x_{t+\tau}^2 = (x_t + \epsilon_t)^2 \tag{13}$$

$$= x_t^2 + 2x_t\epsilon_t + \epsilon_t^2. \tag{14}$$

Averaging over many realizations of the process yields

$$\langle x_{t+1}^2 \rangle = \langle x_t^2 \rangle + 2\langle x_t \epsilon_t \rangle + \langle \epsilon_t^2 \rangle. \tag{15}$$

We first note that $\epsilon_t = \pm a$ implies $\epsilon_t^2 = a^2$, so that $\langle \epsilon_t^2 \rangle = a^2$. Then, given that ϵ_t is statistically independent of x_t, one has $\langle x_t \epsilon_t \rangle = \langle x_t \rangle \langle \epsilon_t \rangle = 0$. As a result,

$$\langle x_{t+\tau}^2 \rangle = \langle x_t^2 \rangle + a^2 \tag{16}$$

so that, assuming $x_0 = 0$, one eventually obtains

$$\langle x_t^2 \rangle = \frac{a^2}{\tau}\, t, \tag{17}$$

which means that the mean square displacement is linear in time. This property is an important feature of random walk, called diffusive behaviour. To emphasize the non-trivial character of this property, let us indicate that the typical distance travelled by the walk after time t is given by $\sqrt{\langle x_t^2 \rangle}$, and is thus proportional to $\sqrt{t}$, which at large time is much smaller than the distance $v_0 t$ travelled by a particle moving at constant velocity v_0.

In the continuous time case, the random walk is characterized by transition rates $W(n \to n-1) = W(n \to n+1) = 1/2\tau$, and $W(n \to n') = 0$ if n' is different from $n \pm 1$. A detailed statistical description of the random walk is then obtained from the corresponding master equation, which reads

$$\frac{dP_n}{dt} = \frac{1}{2\tau}(P_{n+1} + P_{n-1} - 2P_n) \tag{18}$$

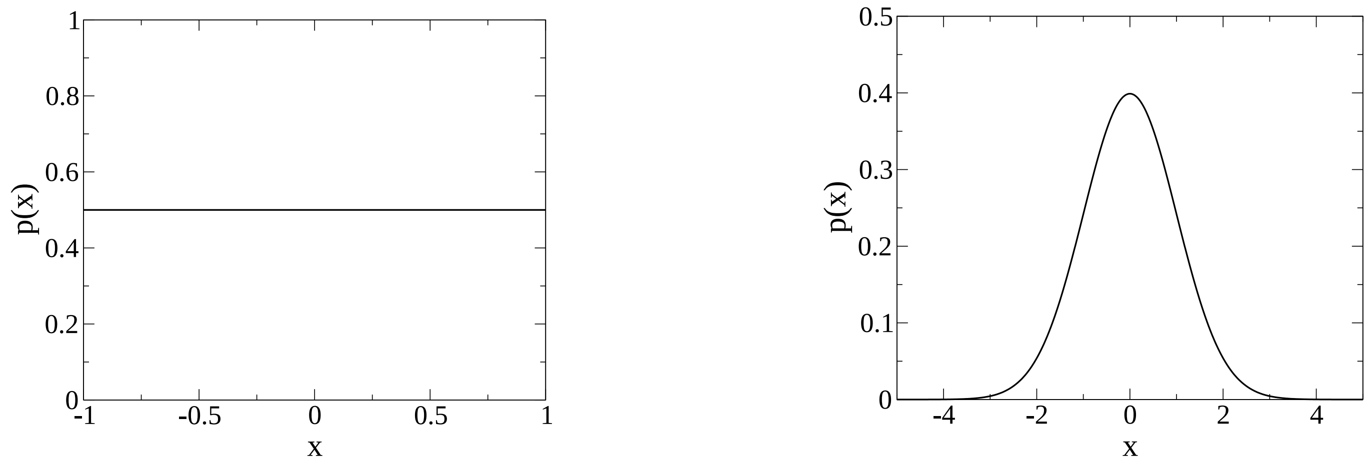

FIG. 2: Illustration of the large-time behaviour of the probability profile of the random walk. Left: diffusion on the finite segment $[-1,1]$. Right: diffusion on an infinite line, in the absence of confining boundaries.

where $P_n(t)$ is the probability to be at position n at time t. At large times, the probability profile appears essentially continuous, and can be approximated by a continuous space equation. Introducing the variable $x = na$ (with a the lattice spacing) and a function $p(x,t)$ of the real variable x satisfying $P_n(t) = a\,p(x,t)$, one obtains the following continuous description, valid for times much larger than the microscopic time constant τ:

$$\frac{\partial p}{\partial t} = D\,\frac{\partial^2 p}{\partial x^2}. \tag{19}$$

This equation is called the diffusion equation, and also appears in other fields of physics, like the diffusion of heat in a material. The quantity $D = a^2/2\tau$ is called the diffusion coefficient.

At very long time, the probability profile depends on the boundary conditions. If the walk is confined on a finite segment, the probability $p(x,t)$ tends to a spatially uniform distribution on this segment when the time t goes to infinity (left panel of Fig. 2). In contrast, if the walk diffuses on an unbounded domain, it converges to a Gaussian shape that keeps broadening as time elapses, as seen on the right panel of Fig. 2.

Interestingly, this Gaussian shape of the distribution, found by solving Eq. (19), can also be given an alternative interpretation. Starting from the discrete time formulation of the random walk given in Eq. (12), one can reexpress x_t as a sum of random variables according to

$$x_t = \sum_{t'=0}^{t-1} \epsilon_{t'}\,. \tag{20}$$

One can then apply the Central Limit Theorem, which states that the sum of a large number of independent and identically distributed random variables are distributed according to a Gaussian distribution with a variance proportional to the number of terms. One thus precisely recovers, without any extra calculation, the result obtained above by solving the diffusion equation Eq. (19).

Before concluding this brief introduction to the stochastic formalism, it is worth mentioning a slight generalization of the diffusion equation, called the Fokker-Planck equation. This equation describes the case when the random walk is not necessarily symmetric, that is the probabilities to go to the left and to the right are not necessarily equal. This situation can be formulated mathematically as follows. One considers a discrete time random walk defined by the recursion relation $x_{t+1} = x_t + \epsilon_t$, where $\epsilon_t = +a$ with probability $\frac{1}{2}(1+aq_n)$, and $\epsilon_t = -a$ with probability $\frac{1}{2}(1-aq_n)$. Denoting $q_n = Q(na)$ and using arguments similar to the ones considered above to derive the diffusion equation (19), one obtains the following Fokker-Planck equation:

$$\frac{\partial p}{\partial t}(x,t) = -\frac{\partial}{\partial x}\Big(2D\,Q(x)\,p(x,t)\Big) + D\,\frac{\partial^2 p}{\partial x^2}(x,t). \tag{21}$$

This equation turns out to be useful in many different modelling contexts, from physics to chemistry and biology [3].

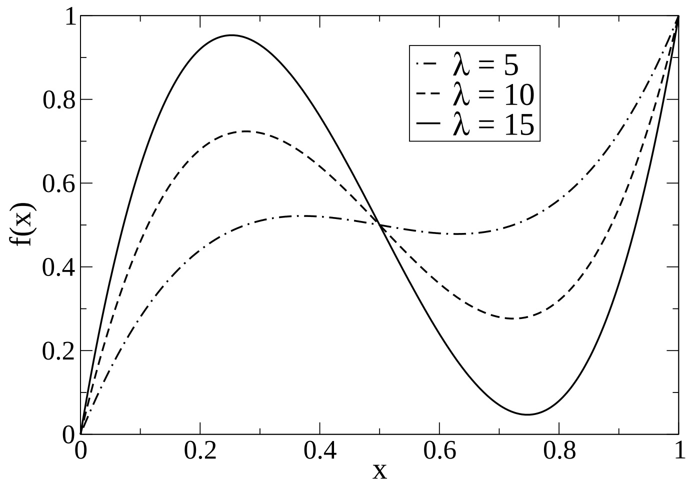

FIG. 3: Illustration of the shape of the function $f(x)$ for $\lambda = 5$ (dot-dash), $\lambda = 10$ (dashed line) and $\lambda = 15$ (full line).

III. DETERMINISTIC DYNAMICS: FROM REGULARITY TO CHAOS

A. A simple deterministic process

We now turn to the study of deterministic processes, with the aim to compare them to stochastic processes under some circumstances. A time signal is considered as deterministic if the knowledge of the value $x(t)$ of the variable considered determines the value $x(t')$ of the variable at any later time $t' > t$. A standard mathematical formulation for continuous time deterministic processes is the following type of differential equation

$$\frac{dx}{dt} = F\big(x(t)\big). \tag{22}$$

In the case of discrete time processes, one rather has:

$$x_{t+1} = f(x_t). \tag{23}$$

Note that the discrete time case can be seen as a periodic sampling of a continuous time process. In this case, the function $f(x_t)$ can be obtained by integrating the differential equation (22) between times t and $t+1$.

A simple and illustrative example is provided by the discrete time deterministic process $x_{t+1} = f(x_t)$, with the function $f(x_t)$ given by

$$f(x) = x\left[\lambda\left(x - \frac{1}{2}\right)(x-1) + 1\right]. \tag{24}$$

The function $f(x)$ depends on a parameter λ, and its shape is illustrated in Fig. 3 for three different values of λ.

The behaviour of the deterministic process $x_{t+1} = f(x_t)$ is illustrated on Figs. 4 and 5 for different values of λ. For $\lambda = 5$, a fast convergence to a fixed point, such that $x = f(x)$, is observed (left panel of Fig. 4). Raising λ, a different behaviour is observed: for $\lambda = 10$, the process converges to a limit cycle, corresponding to the oscillation between two distinct values of x (right panel of Fig. 4). Further increasing λ, a second qualitative change of behaviour appears, as seen for $\lambda = 15$. Here, no regular pattern is observed, and the process becomes chaotic, as seen on the left panel of Fig. 5. Extending the time window (right panel), one sees that the irregular behaviour is indeed a stationary feature, and not simply a transient effect.

Note that this transition from fixed points to chaotic behaviour through limit cycles when varying the control parameter is believed to be a generic scenario for the transition to chaos [4].

B. Chaotic walk

As discussed in section II, a paradigmatic stochastic model is the random walk, which has many applications in different fields. It is interesting to observe that the above chaotic map can be used to define a simple deterministic analog of the random walk, namely a chaotic walk [7].

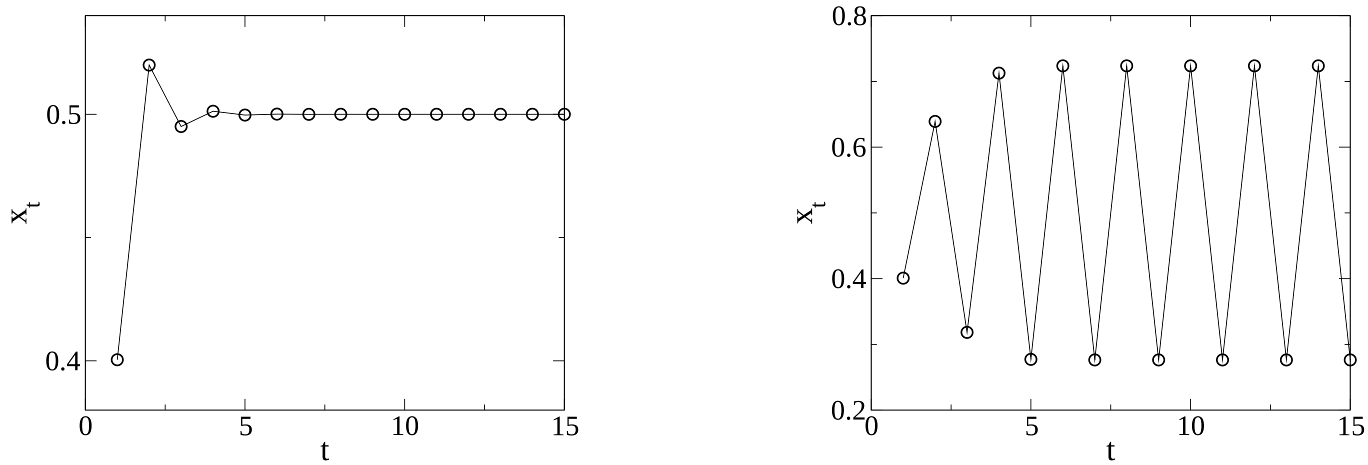

FIG. 4: Left: Convergence to a fixed point for $\lambda = 5$. Right: Convergence to a limit cycle (oscillation between two different points) for $\lambda = 10$.

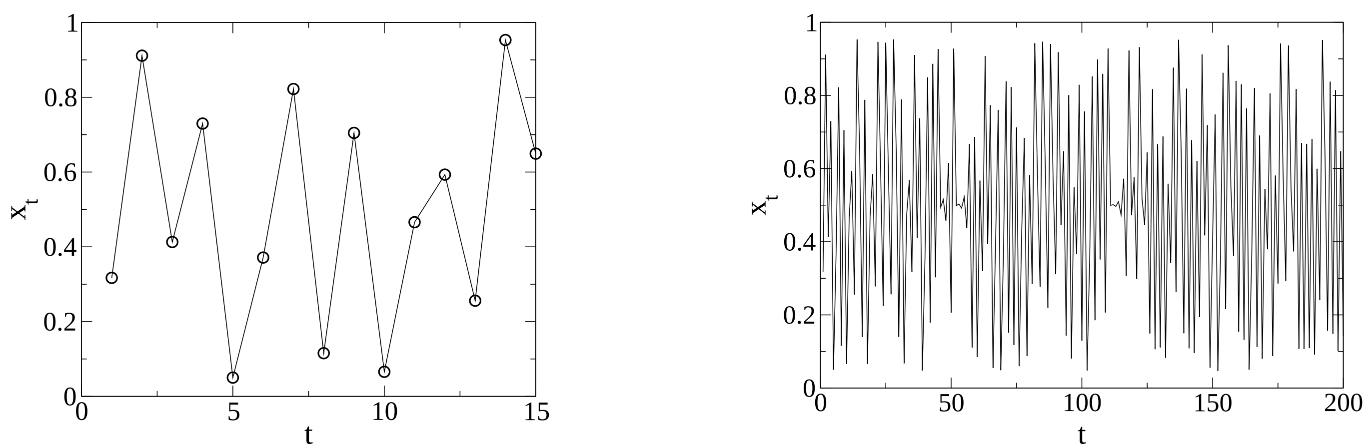

FIG. 5: Case $\lambda = 15$, showing a chaotic behaviour. Left: Same time window as on Fig. 4. Right: Larger time window.

Let us start by introducing a variable u_t evolving according to

$$u_{t+1} = f(u_t), \qquad 0 \leq u_t \leq 1, \tag{25}$$

where $f(u)$ is the function defined in Eq. (24). The idea is now to use the chaotic variable u_t as the increment of a walk, namely

$$x_{t+1} = x_t + (2u_t - 1). \tag{26}$$

Note that, more precisely, the increment $(2u_t - 1)$ is used instead of u_t in order for the increment to take values between -1 and 1, that is, on a symmetric interval around 0. The chaotic walk is illustrated in the left panel of Fig. 6. The visual similarity with a random walk, shown for comparison, is clear. A closer look however reveals a short time anticorrelation in the chaotic walk: positive increments are more likely to be followed by negative increments than by positive ones.

A more quantitative comparison is obtained by computing the mean displacement $\langle x_t \rangle$ and the mean square displacement $\langle x_t^2 \rangle$. Average values are obtained as ensemble averages, that is by averaging over a large set of trajectories obtained by varying the initial conditions (averages are thus time-dependent). Here, the initial position is fixed to $x_0 = 0$, and the initial increment u_0 is sampled in a uniform way from the interval $(-1, 1)$. Note that the sampling is deterministic, that is, equidistant values on the interval $(-1, 1)$ are chosen. The resulting mean displacement $\langle x_t \rangle$ is found to be almost equal to zero, up to the measurement uncertainty, as seen on the right panel of Fig. 6. The mean square displacement $\langle x_t^2 \rangle$ is found to be linear in time, as would be the case for a random walk. Hence, one sees that such simple and standard indicators as mean and mean square displacements cannot be used to discriminate between

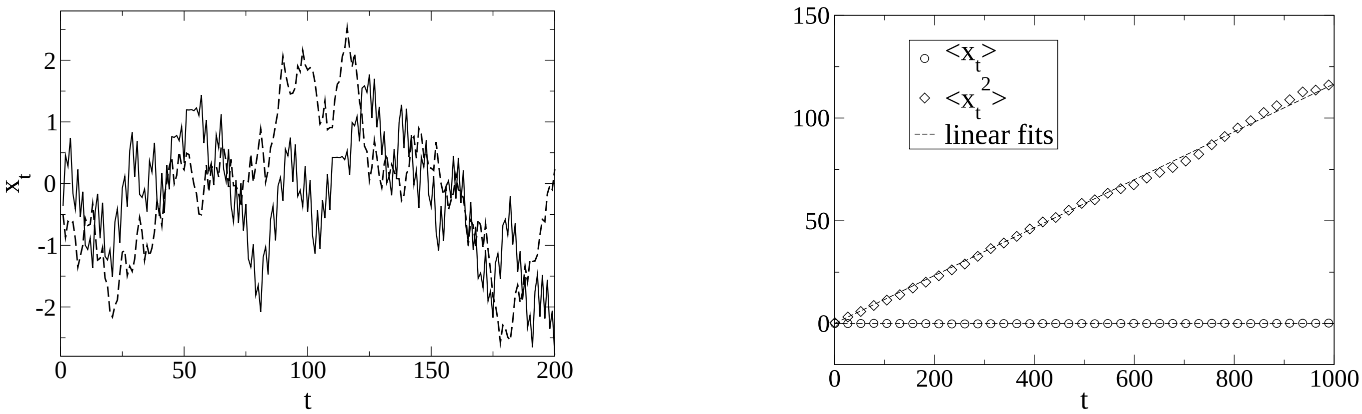

FIG. 6: Left: Chaotic walk (full line); a random walk (dashed line) is shown for comparison. Right: Mean displacement $\langle x_t \rangle$ and mean square displacement $\langle x_t^2 \rangle$ of the chaotic walk, obtained by averaging over many trajectories having different initial conditions. The obtained results are very similar to the results that would be obtained for a random walk.

chaotic and deterministic signals. In addition, it also suggests that from a practical perspective, the distinction between the deterministic or stochastic character of a signal might not be so important. Indeed, if a deterministic system generates a signal similar to the above chaotic walk, why not modeling it as a random walk? This very question is the topic of the next section.

IV. STOCHASTICITY VS. DETERMINISM: A CHOICE OF DESCRIPTION?

Let us come back to the map $x_{t+1} = f(x_t)$ studied in section III A. Instead of simply computing a few average values, a richer information is obtained by determining the histogram of the values of x_t. The resulting histogram is shown on the left panel of Fig. 7, in the case $\lambda = 15$ where the dynamics is chaotic.

As usual, the histogram is build by splitting the interval $(0, 1)$ into a certain number of bins, and by counting how many values of x_t fall into a given bin, along the trajectory. Now it is interesting to note that the dynamics is deterministic on condition that the value of x_t is known with an infinite precision. However, in practice, only a finite precision on the data is available. To illustrate this issue, let us consider that we use the above bins not only to determine the histogram, but also to simulate the dynamics of x_t, that is, to define the "microscopic" configurations of the process. Then, in terms of bins, the dynamics can no longer be considered as purely deterministic, as the value of x_t in a given bin can evolve into different bins as time elapses. In other words, the choice of an initial bin is not enough to determine the occupied bin at any later time.

An effective stochastic dynamics can then be defined in the following way. First, we measure the transition probability $T(j \to k)$ from any bin j to any bin k in a single time step ('probability' is here understood as a frequency of occurrence –see the paper by J. Velasco in this Special Issue). Then, in a second step, we simulate a stochastic process defined by the transition probabilities $T(j \to k)$ measured in the coarse-grained deterministic process. The histogram of this stochastic process can also be measured, and can be compared with the original histogram of the deterministic dynamics (see Fig. 7). A striking similarity is observed, showing again that in practical situations, it may be hard to distinguish a stochastic process from a deterministic one. Though this result might be understood as a negative statement, such a property also has some advantages, as it might be convenient in some cases to model a deterministic process by a stochastic one.

There are however more sophisticated ways to try to distinguish between a deterministic (chaotic) and random signals. One can look for instance for the dimension of the underlying attractor (the generalization of the notion of fixed points, having zero dimension, or of limit cycle, having dimension one), assuming implicitly the process to be deterministic. The dimension found for a stochastic process would then in principle be infinite. However, as for the other (more naive) indicators discussed above, the stochastic or deterministic nature of a process may remain very difficult to assess on the basis of real data, which basically consist in a finite set of points. With this issue in mind, some authors have formulated the interesting proposition to classify the behaviour of a signal as "stochastic or deterministic on a certain scale of resolution" [8].

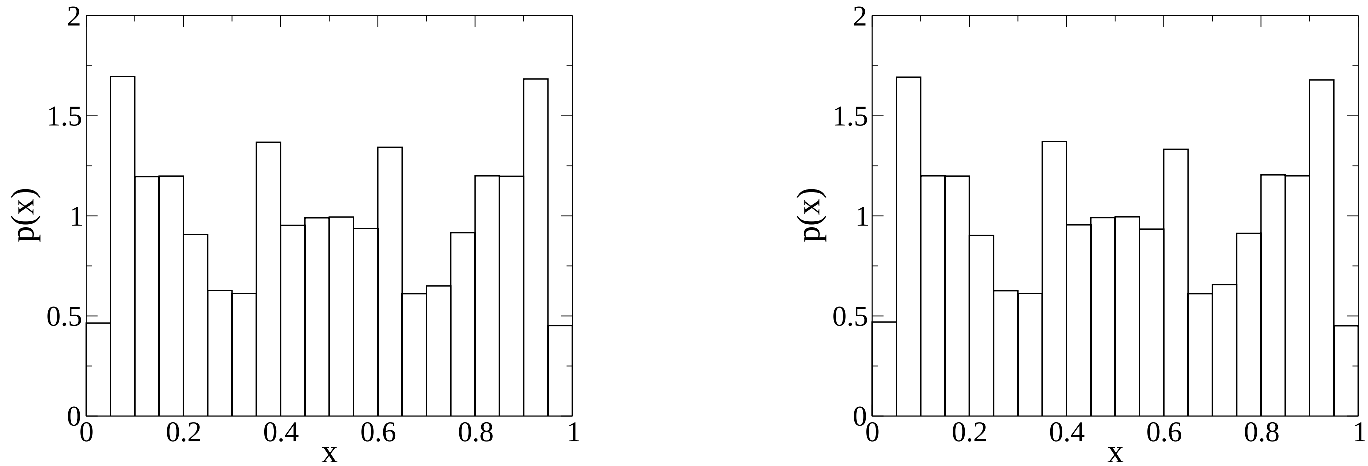

FIG. 7: Left: Histogram of the values of x_t, using the deterministic evolution $x_{t+1} = f(x_t)$, in the case $\lambda = 15$. Right: Histogram obtained from the effective stochastic process mimicking the deterministic one (see text). Both histograms are hardly distinguishable.

V. CONCLUSION

As a summary, we have tried to give in these notes a brief pedagogical account of some similarities and differences between stochastic and deterministic processes, providing along the way a short presentation of some basic notions on the mathematical description of stochastic processes. Our aim was to illustrate that the gap between the behaviour of stochastic and deterministic processes might, quite surprisingly, be much smaller than a priori expected.

Let us emphasize that there indeed exists an absolute distinction, at the conceptual level, between deterministic and stochastic processes. These two types of processes obey different types of laws or equations, and can thus be distinguished without ambiguity when dealing with the mathematical formalism. However, from a practical perspective, that is when dealing with real data (either coming from a real-world experiment, or from numerical simulations), one has to cope with the finite resolution of the data, and the distinction between stochasticity and determinism becomes blurred –at least on the basis of the sole data. Of course, it may also be known that the data were obtained through a deterministic numerical simulation, but this knowledge constitutes an extra piece of information, not contained in the data themselves. Hence, to some extent, determinism or stochasticity are, at a practical level, choices of description ("do I use a deterministic or a stochastic model to describe a given real system?")

As a final remark, let us also note that even at a conceptual level, determinism and stochasticity are notions that apply only to *mathematical descriptions*, that is, to models of the real world, and not to the real world itself. It is thus not clear if asking whether some data obtained from a real-world experiment are intrinsically deterministic or stochastic is a meaningful question. One should probably rather ask which type of model, deterministic or stochastic, is the more relevant to describe the data.

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